Accurate Numerical Simulations of Chemical Phenomena Involved in Energy Production and Storage Using MADNESS and MPQC

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Codes

MADNESS Project Page:

code.google.com/p/m-a-d-n-e-s-s/

MPQC Project and Download Pages:

www.mpqc.org
sourceforge.net/projects/mpqc/

LIBINT Download Page:

www.chem.vt.edu/chem-dept/valeev/software.html

All three codes are licensed under the GPL.

Project Overview I

Simulation of chemical processes for a cleaner world:

Industrial Catalysis

Fuel Reprocessing

Project Overview II

Simulation of chemical processes for a cleaner world:

Energy Conversion

Energy Storage

Computational Approach, Numerical Methods

- **Hybrid programming model:** Both codes are designed to use MPI+Threads, utilize asynchronous communication and already scale to more than 100K cores.
- **Composable software:** Advanced programming techniques are exploited for rapid development. MADNESS striving to minimize syntactic discrepancy between math and code.
- **Novel numerics:** MADNESS using an adaptive multiwavelet representation and exploits low-rank properties of operators to achieve unprecedented precision at *lower* computational cost than traditional methods. MPQC provides explicitly-correlated (R_{12}) methods, which converge rapidly compared to traditional methods.

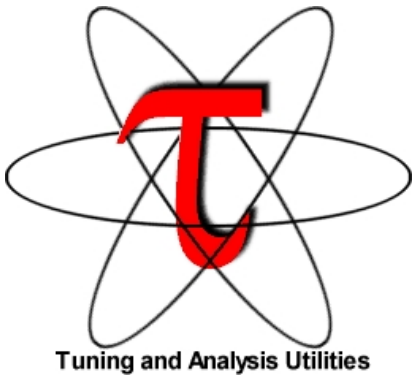
Library and Tool Dependencies

Libraries

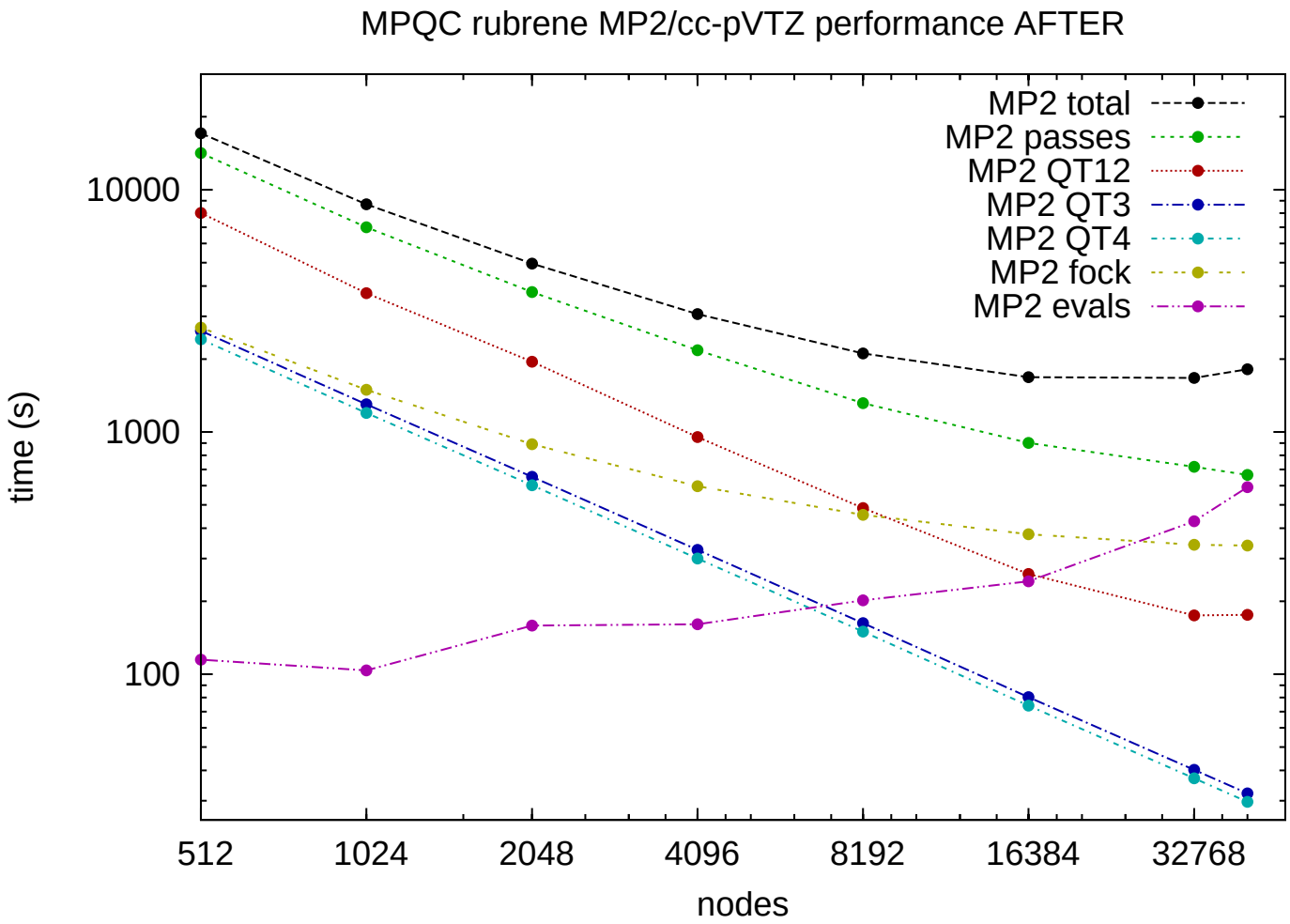
- BLAS, LAPACK, OpenMP, Pthreads, MPI
- PAMI active-messages
- Intel Threading Building Blocks (TBB)
- Boost

Tools

- C++ compilers, Python
- Autotools, SVN, Git, Mercurial
- TAU, debuggers
- Google test and perftools



Scaling of MPQC on Blue Gene/P



Anticipated Modifications for Blue Gene/Q

- **Hybrid programming model:** Both codes already use MPI between nodes and Pthreads within the node. Need to add OpenMP for fine-grain parallelism. Mixing thread models complicates things.
- **Dynamic load-balancing:** MADNESS load balancing initially by work stealing and then by hypergraph partitioing (DAG) will be done as part of the project.
- **Kernel tuning:** MADNESS kernels needs to be optimized in assembly and threaded. Vectorization of MPQC integral codes required for efficiency.
- **Scalable algorithms:** Dense linear algebra is fundamental to quantum chemistry, required for SCF/DFT diagonalization as well as orbital localization. Scalability is now more important than efficiency.

Plan for Next 6 Months Effort

Libraries and tools

- Port TBB and Google tools to BG/P
- Continue working with IBM on BG/Q threading models

Application software development

- BG/P vectorization and OpenMP in kernels
- MPI-IO in MPQC many-body methods
- Further testing of MADNESS on BG/P
- Explore active-messages for MadRT and LibSC

Staffing

ESP postdoc candidate has already been identified.